Allocations & Job Accounting

As part of applying for a NAS account, you (or your principal investigator) requested an allocation for computing time on HECC systems. Allocations for NAS supercomputing resources are granted per project group ID (GID), and are specified in <u>standard billing</u> units (SBUs).

Usage Charge Methods

System usage is charged as follows:

- **Front-End Systems**: Usage is *not* charged on the Pleiades front-end systems (PFEs). However, remember that these front-end nodes are intended for editing and/or compiling and running short testing jobs—not for running production jobs. If you misuse these systems, your jobs will be terminated.
- Lou Data Analysis Nodes: Usage is not charged on the Lou data analysis nodes (LDANs), which provide dedicated PBS resources for pre- and post-processing tasks.
- **Compute Nodes**: Usage on the Pleiades, Aitken, Electra, and Endeavour compute nodes is charged. The number of SBUs charged to a job is calculated by multiplying the number of total wall-clock hours used by the minimum allocation units (MAUs) —the smallest unit of hardware resource that the Portable Batch System (PBS) will allocate to a job.

SBU rates vary by processor type and system. See <u>lob Accounting</u> for a full list.

To continue running jobs after your SBU allocation has been expended, you will need to request more hours. You can check your remaining SBU balance by running the acct_ytd command. See <u>Job Accounting Utilities</u> for more information.

TIP: You can easily keep track of allocation and usage for all of your GIDs (and monitor all of your PBS jobs) in one central location by logging into the myNAS Portal.

Charging to a Non-Default GID

If you have access to more than one GID, only one of those GIDs is set as your default. The default GID is listed in the/etc/passwd file of each system you have access to. Your jobs will be charged to the default GID unless you specify a different one. If you want to charge your usage to a non-default GID (for example, s0901), add the GID to your PBS script. For example:

#PBS -W group list=s0901

Understanding Queues

All HECC supercomputers use the Portable Batch System (PBS) to manage both interactive and batch jobs. Pleiades, Aitken, and Electra use the same PBS server and job submission queues. Endeavour has a separate PBS server and separate queues.

Although different queues are available on different systems, queues typically have constraints on maximum wall-clock time and/or the number of nodes allowed for a job. Some queues have other constraints or are restricted to serving certain users or GIDs. In addition, mission directorate limits are set on the number of cores available on Pleiades, Aitken, and Electra to ensure that each mission directorate can access a fair share of resources.

You can use the qstat command as follows to view various types of information:

qstat -Q

Lists available queues and their constraints on a system.

qstat -Qf

Lists available queues and their constraints on a system.

qstat -W shares=

Lists mission shares available for each mission.

For more information, see the following articles:

- PBS Job Queue Structure
- Mission Shares Policy

Usage on HECC compute systems is charged using a <u>standard billing unit (SBU)</u>. SBUs are charged to each PBS job running on the compute nodes according to the following formula:

SBUs charged = wall-clock hours used * number of MAUs * SBU rate

where MAU represents the minimum allocatable unit of resources available through PBS.

On Aitken, a MAU is a node with 40 cores (Cascade Lake) or 128 cores (Rome). On Electra, a MAU is a node with 28 cores (Broadwell) or 40 cores (Skylake). On Pleiades, a MAU is a node with 16 cores (Sandy Bridge), 20 cores (Ivy Bridge), 24 cores (Haswell), or 28 cores (Broadwell). On Endeavour, a MAU is a socket with 28 cores (Cascade Lake).

Charges are based on the number of MAUs allocated to a job, not how many cores are actually used during runtime. Once a user is allocated the resources, that user has exclusive access to those resources until the user's job completes or exceeds its requested wall-clock time.

Note: Usage of the front-end systems (PFEs and SFEs) and the Lou data analysis nodes (LDANs) is not charged.

The following table shows the SBU rates for each processor type:

Host		SBU Rate
Aitken	Rome	4.06
	Cascade Lake	1.64
Electra	Skylake	1.59
	Broadwell	1.00
Pleiades	Broadwell	1.00
	Haswell	0.80
	lvy Bridge	0.66
	Sandy Bridge	0.47
	GPU (4 V100s)	9.82
	GPU (8 V100s)	15.55
Endeavour	Cascade Lake	1.31

On Endeavour, charges apply both to jobs that run successfully and those that are interrupted. Interrupted job charges are calculated by subtracting 1 hour from the elapsed job time, then multiplying the total by the number of MAUs used. Users are encouraged to have their applications checkpoint roughly every hour.

For example, if you submit a 24-hour job on Endeavour that requires 16 MAUs (448 cores) and the job stops unexpectedly after running 12 hours, your allocation will be charged. The accounting system will subtract 1 hour from the 12 hours the job ran, and compute the SBUs as follows: $11 \text{ hours } \times 16 \text{ MAUs } \times 1.31 = 230.56 \text{ SBUs}$.

Common Standard Billing Unit (SBU)

A common Standard Billing Unit (SBU) normalizes computing time usage across different types of processor architectures, and is used for allocating and tracking usage for both the HECC project and the NASA Center for Climate Simulation (NCCS).

For details about the charging formula and SBU rates for each processor type, see the <u>Standard Billing Units</u> policy on the NASA High-End Computing Program website.

Charging to a Project Group ID (GID)

Each approved project is assigned a group ID (GID). Members of a GID are authorized to use the resources allocated to that GID. For those users who have access to multiple GIDs, be aware that only one of those GIDs is considered your default.

Use the groups command to find which GIDs you are a member of. The following example shows that user zsmith is a member of the groups a0800, a0907, all, and e0720.

%groups zsmith

zsmith: a0800 a0907 all e0720

The first GID from the "groups" list should be your default GID. This can be verified through the/etc/passwd file. For example, the /etc/passwd file has an entry for user zsmith with the GID 20800 (which is the same as a0800, his default GID).

%grep zsmith /etc/passwd

zsmith:x:6666:20800:Z. Smith,,650-604-4444,:/u/zsmith:/bin/csh

When you use resources on the compute nodes through PBS jobs, SBUs are deducted from your default GID unless you specify otherwise. To charge resource usage to an alternative GID for a batch job, you can use the PBS flag -W group_list=account either in your script or on the qsub command line. For example:

#PBS -W group_list=a0907

or

%qsub -W group_list=a0907

Mission directorate shares have been implemented on HECC systems for more than ten years. Implementing shares guarantees that each mission directorate gets its fair share of resources.

The share to which a job is assigned is based on the project group ID (GID) used by the job. After all the cores within a mission directorate's share have been assigned, other jobs assigned to that share must wait. This is true even if cores are available in a different mission directorate's share, with the following exception:

When a mission directorate is not using all of its cores, other mission directorates can borrow those cores, but only for jobs that will finish within 4 hours. When part of the resource is unavailable, the total number of cores decreases, and each mission directorate loses a proportionate number of cores.

You can display the share distribution by adding the -W shares=- option to the qstat command. For example:

%qstat -W shares=-

Group Share% Use% Share Exempt Use Avail Borrowed Ratio Waiting

```
Overall 100 0 405070 0 44 405026
                                   0 0.00 47680
       27 28 110166 747 116736 0 6570 1.06 392206
ARMD
        23 21 93560 1360 87952 5608
HEOMD
                                      0 0.94 125004
SMD
       33 33 136088 16 136696 0 608 1.00 390340
        14 7 56703 0 30724 25979
ASTRO
                                    0 0.54 131656
NAS
       2 0 8505
                  0 3080 5425
                                 0 0.36 67488
```

Mission shares are calculated by combining the mission's HECC share of the shared assets with the mission-specific assets. The second column of the sample output above shows the mission shares. Other information displayed includes: the amount of resources used and borrowed by each mission, the amount of resources available to each mission, and the resources each mission is waiting for.

The qs utility (available under /u/scicon/tools/bin/qs) provides similar information, and also includes details that break the resources into the different processor types. In addition, the utility can show the remaining time for jobs that are running, or how much time was requested by waiting jobs.

Specify the -h option of qs for instructions on how to use it. For example:

% /u/scicon/tools/bin/qs -h

```
usage: qs [-d] [-D] [-h] [-M] [-n N] [-o] [-r] [-s svr] [-t] [-u] [-v] [-w]
         [-x] [--audit f] [--file f] [--runout f] [--user U]
            : darker colored resource bars (for a light background)
    -D
            : show count of offline & down nodes
    -h
            : provide this message
    -n NUM : show time remaining before NUM nodes are free
    -N NUM
               : show time remaining before NUM nodes are free; suppress
            other output
            : show old-style resource usage without time information
    -O
            : show runout times & expansion factors
            : show data for PBS server svr [default: pbspl1]
    -s svr
    -t
           : show time remaining & nodes used for each running job
            : highlight resources for jobs of user running qs
    -u
            : (verbose) provide explanation of display elements
    -v
            : have resource bars show wait time, not remaining time
    -W
             (cannot be used with -n, -o, -t, or -x)
            : have resource bars show expansion factor of jobs,
             not remaining time (cannot be used with -n, -o, -t or -w)
    --audit f: reserved for debugging
    --file f : reserved for debugging
    --runout f : put runout information in file f
    --user U : highlight resources for jobs of users U (comma-separated list)
    --noShares: highlight resources for jobs that could start now if no shares
    -- 1 node : highlight resources for jobs that use only 1 node
```

Here is a sample output file of qs:

```
pbspl1:10-Oct-2019 13:07 100% of mission share
ARMD
r:105%
     14335
             :::+325+55555555
w:412%
      .4.55
             :::+325+55555555
            ::::+555+5555555+
      :5:5
            :::5+555+5555555+
      :545
      1:55
            :::5+555+5555555+
      2215
            :::535.525555555+
            :::+35+555555555
      2245
           -running, exempt from share
HEOMD
r: 95%
     .33:
            :;#25+
            :#.55#
w:138%
     +4+#
      352#
            ;#55##
            ;#55#
      4:3:
            ;#55#
      ++.;
            ;#55#
      11.2
           -running, exempt from share
ASTR0
         1
r: 54% 251 +155+2551
w: 233% 52 2+25512521
      54 5+25+225+
SMD
r:100% .;5##
             w:1369% 3++#
            1#4#
            1#1#
      2###
            41##
            51##
            -running- -waiting-
          -running, exempt from share
                                <=1d
                                                   <=4d
Key:
             <=2h
                   <=4h
                         <=8h
                                      <=2d
                                             <=3d
                                                          \leq 5d
                                                                >5d
Pleiades Used Nodes (above) .... san:1544 ivy:4713
                                          has:1929
                                                  bro:1892
                                                          ele:1135 sky:2191 cas:1024
Pleiades Unused Nodes (below)... san: 1 ivy: 0
Unused. but limited by Resv .... san: 0 ivy: 0
                                          has: 1 bro: 4
                                                          ele:
                                                                4 sky: 0
                                                                           cas:
                                                        2 ele:
                                                                0 sky:
                                          has:
                                                0
                                                   bro:
                                                                        0
                                                                           cas:
                                                                                 0
Unused in <u>devel,*ops</u> queues .... <u>s</u>an: 209 <u>i</u>vy: 243 <u>h</u>as: 93 <u>b</u>ro:
Unused GPU Nodes (G,G) ...... 58
                                                          ele:
                                                                   sky:
                                                                           cas:
Unused ldan Nodes (L) ..... san:
Unused ded Nodes (0,0,0,0,0,0,0,0) san: 36 ivy: 53 has: 5 bro: 1 ele: 0 sky: 41 cas: 106
      s <u>i</u> Q
       ib Q
Merope Unused ..... wes: 398
Each letter/number/symbol (w,s,i,h,b,e,k,c,#,#,#,#,#,#,#,#,) ~= the same number of SBUs/hr
(which varies with your window width and current mix of jobs running and queued)
==> in nodes: w,# ~= 354.4 wes; s,# ~= 265.8 san; i,# ~= 212.6 ivy; h,# ~= 177.2 has;
          b,# ~= 151.9 bro; e,# ~= 151.9 bro_ele; k,# ~= 106.3 sky_ele; c,# ~= 106.3 cas_ait nodes.
```

Allocations & Job

You can use the following job accounting utilities to obtain resource usage and charging information for your<u>project group IDs</u> (GIDs):

- Year-to-date summary: acct_ytd
- Detailed account queries: acct_query

TIP: Use the myNAS portal to easily check allocation and usage for your GIDs, as well as monitor your PBS jobs. See <u>Using the myNAS</u> Portal for more information.

The acct_ytd command

The acct_ytd command provides a year-to-date summary of accounting information for the GID groups you belong to, as of the most recent accounting run. Accounts are typically run every night at 12:00 a.m. (Pacific Time).

To view information for each GID you have access to on a host, run the acct_ytd command on that host without any parameters. For example:

% acct_ytd

To view information about a single GID (for example, a0800), specify the GID on the command line:

% acct_ytd a0800

You can also use the -c all option to get allocation and usage information on all NAS systems.

For example:

% acct_ytd -c all a0800

See man acct ytd for more information.

The acct_query command

The acct_query command searches and displays process-level billing records. You can view detailed billing records for each process run during a particular period, total processes run during the period, or total processes for each day in the period.

For example, to view all of your <u>standard billing unit (SBU)</u> usage for the operational year 2019 (defined as Nov. 1, 2018 to Sept. 30, 2019) for all GIDs you have access to on Pleiades:

% acct_query -y19

To view all SBU usage beginning Nov. 1, 2019 and ending Dec. 1, 2019 for all projects user zsmith has access to (-p all, default) and on all hosts (-c all):

% acct_query -b11/01/19 -e12/01/19 -p all -c all -u zsmith

To specify a GID (for example, a0800), replace -p all with -p a0800.

Important: A new SBU rate went into effect on October 1, 2018. One unit of the new SBU rate is equivalent to 3.94 of the previous SBU rate. Keep in mind that for usage prior to October 1, 2018, the acct_query command output shows data measured using the old SBU; for usage after this date, the output shows data measured using the new SBU. Therefore, when you run the acct_query command, your search parameters should not cross October 1, 2018.

Eligible Hostnames for the -c Option

You can use any of the following parameters after the -c option in the $acct_query$ command line:

- all (includes all Pleiades, Aitken, Electra, and Endeavour processor types, and cloud)
- aws (for AWS cloud)
- cloud-all (for all cloud types; currently, just AWS cloud)
- hecc-all (default; includes all processor types except cloud)
- par-all (same as hecc-all)
- aitken C (for Aitken Cascade Lake nodes)
- aitken_R (for Aitken Rome nodes)
- electra_B (for Electra Broadwell nodes)
- electra_S (for Electra Skylake nodes)
- endeavour1 (for Endeavour node usage prior to March 31, 2021)
- endeavour2 (for Endeavour node usage prior to March 31, 2021)
- endeavour3
- endeavour4
- e-multi (for jobs that ran across Endeavour1 and Endeavour2)
- pleiades (for Harpertown node usage prior to Aug. 2013)
- pleiades_N or pleiades_ch1 (for Nehalem node usage prior to Aug. 2014)
- pleiades W or pleiades ch2 (for Pleiades Westmere usage prior to June 2016)
- pleiades_S or pleiades_ch3 (for Sandy Bridge nodes)

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- pleiades I or pleiades ch4 (for Ivy Bridge nodes)
- pleiades_H or pleiades_ch6 (for Haswell nodes)
- pleiades_B or pleiades_ch7 (for Pleiades Broadwell nodes)
- pleiades_MH or pleiades_ch5 (for Merope Harpertown usage prior to Aug. 2014)

When you specify multiple users (for example, -u zsmith -u jbrown), you can obtain a summary for each user at the end of the output by adding the -U option to the command line. For example:

% acct_query -y18-p all -c all -u zsmith -u jbrown -U

See man acct_query for more information.

TIP: A space between the option and argument is not required in theacct_ytd or acct_query command lines. For example, acceptable syntax includes both -c all and -call.

The myNAS web portal provides a central location where you can easily monitor all aspects of your NAS user account activity, including PBS jobs, resource allocations, and usage for the project group IDs (GIDs) you belong to. If you use the Shift tool to transfer your data, you can also check the status of your file transfers.

If you are a principal investigator (PI), you will see information about jobs and usage by all users who are assigned to your GIDs.

Follow this link to access the myNAS web portal: https://portal.nas.nasa.gov

Note: You will log into myNAS via NASA's Access Launchpad, using your NASA Smartcard or RSA SecurID token.

Home Page: Information at a Glance

Once you log in, myNAS will automatically load information for your NAS user account. On the home page, you will see:

- The number of jobs currently in each state (running, waiting, recently finished, and held)
- All of your jobs that recently changed state
- The status of your Shift file transfers
- · An estimate of today's usage for each of your GIDs
- The latest HECC news and announcements
- · Scheduled downtimes for all HECC resources

For more detailed information about all of your jobs, click Jobs in the navigation panel on the left side of the page. To check allocation and usage, click Accounts.

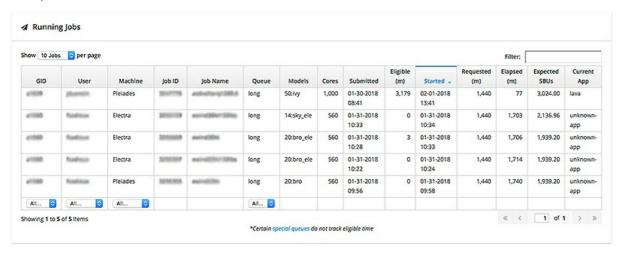
TIP: Take a quick feature tour of each myNAS page by clicking the question mark icon in the top right corner.

Jobs Page: Detailed Job Information

The Jobs page provides details about each of your running, waiting, recently finished, and held jobs, including:

- · GID, job ID, and job name
- Requested queue, machine, processor model, and number of cores
- Date/time submitted, date/time started, and requested and elapsed time
- Number of standard billing units (SBUs) the job is expected to use
- Information about interrupted jobs, if applicable

You can easily sort the tables by column and filter by any text string such as partial job name, model type, machine, and so on. For example:

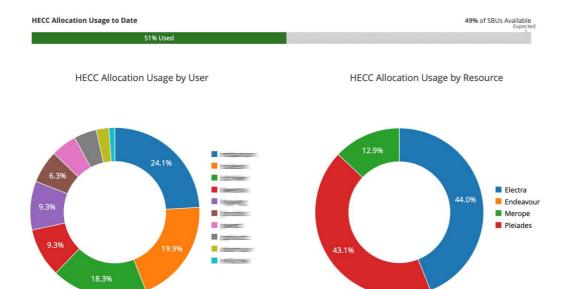


Accounts Page: Detailed Allocation and Usage Information

The Accounts page provides information about all your GIDs, such as PI, project name, mission, and allocation, expected usage to date, and actual usage.

Click the arrow in the left column of any GID listed in the table to see interactive charts that provide allocation and usage information at a glance. The thermometers show overall allocation usage for the GID, while the first donut chart shows either your own usage (if you are an individual user) or usage for all GID members (if you are a PI). The second donut chart shows usage for the GID by resource (machine). For example:

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Continuous Monitoring

We recommend bookmarking the myNAS website in your browser, and taking some time to explore all of the useful information that is available at a glance via interactive tables and charts. Once you are logged in, you can keep the browser window open to easily monitor your job and account activity.